Astrophysics Research And Analysis

Three-dimensional off-lattice Monte Carlo simulations of interstellar grain-surface chemistry and ice structure

Completed Technology Project (2015 - 2017)

Project Introduction

Interstellar dust-grain surfaces are the site of the formation of some of the most important interstellar molecules, such as H_2, H_2O, CH_3OH (methanol), and a range of more complex organic species. This grain-surface chemistry results in the build-up of thick ice mantles around the grains. The accurate interpretation of infrared ice absorption-line data from past instruments such as Spitzer and the upcoming James Webb Space Telescope depends on an understanding of the chemical and physical structure of the ices, as well as their chemical composition. Simulations of dust-grain chemical kinetics provide the bridge between laboratory experiment and space-based infrared observations. However, most simulations of grain-surface and ice chemistry include minimal structural information; averaged chemical reaction rates are used to follow the evolution of chemical abundances, but the exact positions of individual atoms and molecules cannot be traced by such means. While these simple methods are necessary for simulations of environments that are dynamically variable, they can never be used to predict or explain microscopic ice structure and the chemical and observational implications flowing therefrom. Here, a new off-lattice Monte Carlo chemical kinetic model of dust grain-surface chemistry will be used to trace the motions of individual atoms and molecules on the grain surfaces, allowing a precise picture of ice formation, structure and composition. Published preliminary models have demonstrated the feasibility of the project. The model allows the size, shape, and structure of the underlying grain to be specified, atom-by-atom. The model calculates local potential minima on the fly, as surface diffusion occurs; thus the ice forming on the grain surface is not limited to a pre-determined structure, and ice structures build up naturally, based on physical principles. Ray-traced videos can be used to visualize the developing dust-grain ice. The possibilities for investigation include: the degree of porosity in interstellar and laboratory ices; the influence of differing grain sizes, shapes, and surface topologies on grain chemistry; chemical segregation of the ices into polar/apolar components; and the reproduction and parameterization of laboratory ice-chemistry experiments. The new simulation method will be critical to our full understanding of the interaction between interstellar surface chemistry, ice structure, grain morphology, and gas-phase abundances.

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Organizational Responsibility

Responsible Mission Directorate:

Science Mission Directorate (SMD)

Responsible Program:

Astrophysics Research and Analysis

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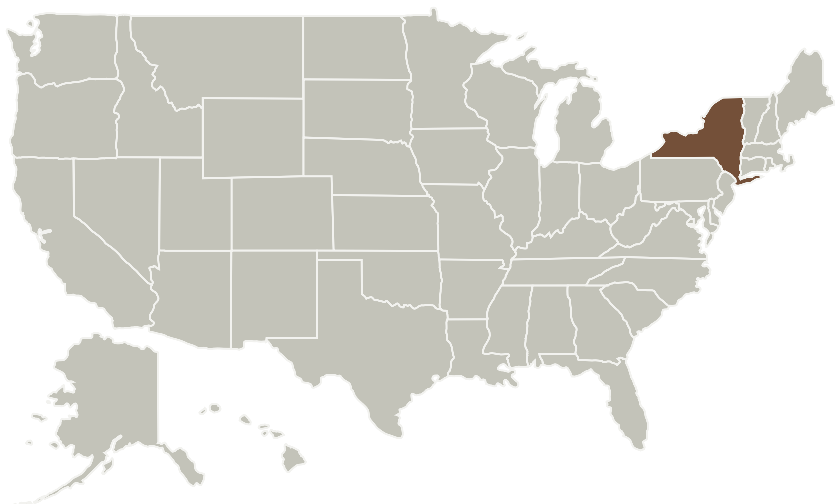
Primary U.S. Work Locations and Key Partners



Organizations Performing Work	Role	Type	Location
Cornell University	Supporting Organization	Academia	Ithaca, New York
Office of Sponsored Programs - Cornell(OSP)	Supporting Organization	Academia	Ithaca, New York

Primary U.S. Work Locations
New York

Project Management

Program Director:
Michael A Garcia

Program Manager:
Dominic J Benford

Principal Investigator:
Robin T Garrod

Technology Areas

Primary:

- TX01 Propulsion Systems
  - └ TX01.3 Aero Propulsion
    - └ TX01.3.11 Engine Icing

Target Destination

Outside the Solar System